

Atomistic Simulations of Chemical Reaction in Nanolaminates under Shock Loading

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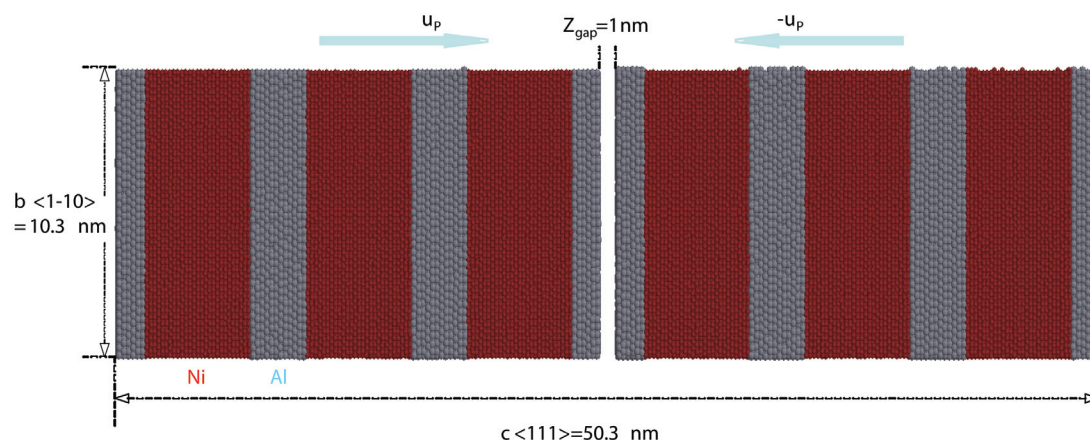
Nanostructured metastable intermolecular composites (MICs) are mixtures of nanosized particles of reactants that undergo exothermic (e.g., thermite) reactions triggered by an external stimulus. This relatively new class of energetic materials exhibits extraordinary properties [1]: extremely fast burn rates, high temperatures and power, accompanied by lower volume expansion than in traditional energetic materials due to the lack of gaseous products. Furthermore, by modifying the nanostructure, such as the particle size, porosity, and passivation layer, one can control the rate of energy release. These unique properties make MIC formulations promising candidates for a wide range of defense and commercial applications, including localized heat sources for chem/bio neutralization and disease treatment, environmentally clean primers and detonators, ultra-fast fuses, and smart thermal barriers. Despite their technological importance, the fundamental molecular-level mechanisms that

govern the extraordinary properties of MICs are unknown; as stated recently [2]: “a lack of understanding of the fundamental mechanisms has hindered the development of nanoenergetic materials.”

In this work, we employ molecular dynamics (MD) simulations to uncover these mechanisms at the atomistic level. We characterize the chemical and mechanical response of nanostructured Ni/Al multilayers induced by shock loading, using a novel technique that captures both the initial shock transit as well as the subsequent longer-timescale chemical processes. In our simulation, two Ni/Al multilayers, originally separated by a 1-nm gap, collide with a relative velocity of $2u_p$ (see Fig. 1). The unequal Ni and Al layer thicknesses are set up such that the final stoichiometry is Ni_3Al , and the interfaces are perfectly planar (111) surfaces. The interatomic interactions are described by an embedded atom method (EAM) potential developed by Mishin et al. [3].

Periodic boundary conditions are imposed in all three dimensions, with a shrinking boundary condition (the left boundary moving at $+u_p$, and the right boundary at $-u_p$) imposed in the $\langle 111 \rangle$ shock direction to maintain that periodicity. (Both the periodic boundary and the central impact plane are located at the midpoint of an Al layer.) Upon collision of the two multilayers, two shock waves (with particle velocity u_p relative to the uncompressed material) propagate outwards in opposite

Fig. 1. Schematic of the simulation geometry. The length in a $\langle 11-2 \rangle$ (the direction perpendicular to the paper) is 8.9 nm. The sample includes $N_{\text{Ni}} + N_{\text{Al}} = 379,080$ atoms with $N_{\text{Ni}} \sim 3N_{\text{Al}}$.



directions, leaving behind a longitudinal particle velocity, which is locally zero in the simulation reference frame.¹ Just at the point when these two shock waves meet at the $\langle 111 \rangle$ periodic boundary, we stop the shrinking boundary condition and begin a constant-volume (NVE) MD run to follow the longer-timescale chemistry initiation and propagation.

Due to the impedance mismatch between the (harder) Ni and (softer) Al layers, the initial shock compression is followed by a complex series of reshocks and rarefaction fans. As these waves move back and forth in the Al and Ni layers, they gradually decay, with characteristic damping rates for each medium [5]. This wave reflection and damping contributes to an additional temperature rise beyond the original shock heating, particularly in the softer Al layers which are increasingly shock-compressed and are heated to a higher temperature than the harder Ni layers (see Fig. 2). The central Al layer (where the initial impact occurred) reaches the highest local temperature because this layer has been subjected to the greatest number and intensity of wave reflections.

Figure 3 shows profiles of the fraction of Al atoms across the nanolayer at various times. We see that chemical reaction begin at the interfaces surrounding the central Al layer, causing a significant decrease in the fraction of Al atoms as Ni diffuses towards the center of the system. The heat generated by these exothermic reactions, as well as further heating due to internal wave reflection, subsequently leads to the initiation of chemistry at interfaces further from the center. In this manner, a reactive wave propagates outwards, with a velocity of approximately 0.1 to 0.2 nm/ps. The highly exothermic alloying reactions propagate in a self-sustained manner by mass and temperature transport, and energy release from chemical reaction at the interfaces [5].

¹Note that in the standard shrinking periodic boundary condition technique [4], the sample is initially at rest and a pair of inward-moving shock waves are generated from the periodic boundary.

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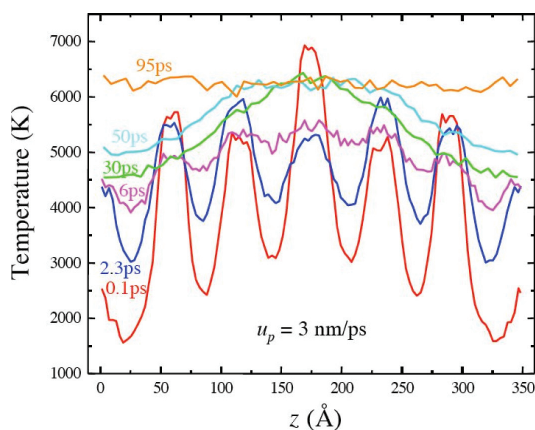


Fig. 2. Temperature distribution along the shock direction (z) at various times, for $u_p = 3$ nm/ps.

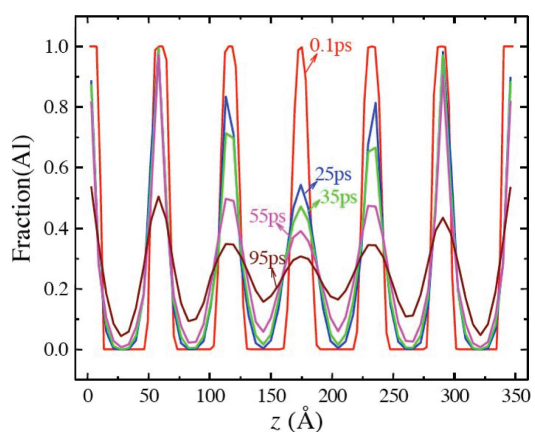


Fig. 3. Al number fraction at various times, indicating chemistry initiation and propagation. The final Al fraction in the central bin has approached a value close to 1/4, the overall Ni_3Al stoichiometry.